

# The Stationary Phase Method for a Wave Packet in a Semiconductor Layered System. The applicability of the method.

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## Abstract

Using the formal analysis made by Bohm in his book, “*Quantum theory*”, Dover Publications Inc. New York (1979), to calculate approximately the phase time for a transmitted and the reflected wave packets through a potential barrier, we calculate the phase time for a semiconductor system formed by different mesoscopic layers. The transmitted and the reflected wave packets are analyzed and the applicability of this procedure, based on the stationary phase of a wave packet, is considered in different conditions. For the applicability of the stationary phase method an expression is obtained in the case of the transmitted wave depending only on the derivatives of the phase, up to third order. This condition indicates whether the parameters of the system allow to define the wave packet by its leading term. The case of a multiple barrier systems is shown as an illustration of the results. This formalism includes the use of the Transfer Matrix to describe the central stratum, whether it is formed by one layer (the single barrier case), or two barriers and an inner well (the DBRT system), but one can assume that this stratum can be comprise of any number or any kind of semiconductor layers.

PACS numbers: 73.23b, 73.40.Gk, 73.40.Kp

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## I. INTRODUCTION

In the last century the calculation of the time spent by a particle when passing through a potential barrier was, for a long time, one of the basic and controversial problems since the early days of Quantum Mechanics. When the issue of the delay time of a transmitted wave packet through a potential barrier was under investigation by MacColl[1] and later by Hartman,[2] using the Wigner's phase time introduced in nuclear physics, the striking superluminal effect arose immediately. At this time the question "how much time does tunnelling take" was loosely formulated.[1] Early answers to this problem [3, 4] and alternative proposals [3, 4, 5, 6, 7, 8, 9] run from pure semiclassical to fully quantum mechanical models. Nowadays the impressive number of low-dimensional semiconductor devices brought a new urgency to the essential measurement and/or modelling of tunnelling time for charge carriers motion. The last can be seen reflected in the large presence of publications.

Early in the '90s, real experiments on photon-twins interference and on optical pulses propagation[10, 11] measured the delay time, in a simple and direct way, at first. On the other hand, most of the available experimental setups, pretending to be relevant to the tunnelling issue, actually involve other times derived from escape and/or decay phenomena. In this sense, their results are not able to identify real tunnelling time scale, and consequently should be questionable as potentially misleading. Authentically connected to the tunnelling process delay measurements,[10, 11, 12] and uncommonly good agreement with some of them,[10, 11] found within the phase-time model,[13] are striking developments from the days of the lively debate on these matters appeared during the late 1980's. Approximate[14] and multiband [15] phase time calculations in different systems, confirm experimental results reported in Ref.[10, 11, 12] and in Ref.[16], respectively. The robustness of the phase time approximation was assured by its consistency with the Maxwell's equations predictions.[17] Being largely stimulated by the success of the phase-time conception, we had applied here the Stationary Phase Method (SPM),[18] firstly to evaluate the phase time as it straightforwardly deals with both initial (incident) and final (transmitted and reflected) dispersion phase amplitudes and finally to further study this magnitude to know its applicability more closely.

In the last years some other authors have studied these problems in many respects.[19, 20, 21, 22] At the same time, in Ref.[19] several references of different applications of the tunnelling process in different low dimensional semiconductor devices are given. This is the reason to further study

this magnitude to know its applicability more closely.

In the present paper the formal analysis of Bohm[3] is used to determine the transmitted wave packet and, properly, the phase time in an arbitrary semiconductor layered system for a charge carrier trespassing the structure. The point is that Bohm got the leading term of the transmitted wave packet and from it, got an expression to calculate the phase time, and these approximations not always are good. To reach when they are good and when do not is our task. The system could be described by a single band or multiband models. In figure 1 the general view of the system under study is depicted, no matter how many layers are included in the group  $M$ .

Using the Transfer Matrix (TM) method,[23] the wave packet reflected and transmitted are obtained, using the SPM[18] to solving the integrals for these waves. This method lead us to an applicability condition for it and, properly, the phase time as a function of the parameters of the system. The application of the resulting expressions for the Schrödinger single band case is given and some results obtained for the double barrier resonant tunnelling semiconductor structure (DBRT) are given for illustration. Some comments were included to extend these results to the case of a system described by  $N$  second order differential system.

## II. THE FORMAL ANALYSIS

In the system depicted in figure 1 the Schrödinger wavefunction can be written as:

$$\psi_o(z, p_R, t) = e^{-iE(p_R)t/\hbar} \phi_o(z, p_R) \quad (1)$$

$$\phi_o(z, p_R) = \begin{cases} D(p_R) \left\| \begin{matrix} 1 \\ i \left( \sqrt{p_R^2 - 2m^*V_{LR}/\hbar} \right) \end{matrix} \right\| e^{iz\sqrt{p_R^2 - 2m^*V_{LR}/\hbar}} + \\ + F(p_R) \left\| \begin{matrix} 1 \\ -i \left( \sqrt{p_R^2 - 2m^*V_{LR}/\hbar} \right) \end{matrix} \right\| e^{-iz\sqrt{p_R^2 - 2m^*V_{LR}/\hbar}} & z < a_1 \\ M(z, a_1 -) \psi(a_1 -, p_R) & a_1 < z < a_2 \\ A(p_R) \left\| \begin{matrix} 1 \\ i(p_R/\hbar) \end{matrix} \right\| e^{ip_R z/\hbar} & z > a_2 \end{cases} \quad (2)$$

where the TM of wavefunction and derivative[24] was included to describe the central layer  $M$ . [23] As this part can be arbitrary, the expression for the TM will depend on the form of the

potential of this layer. Also it was written  $p_R = \sqrt{2m^*E}$ . The wavefunction for the layer  $L$  was also written in terms of  $p_R$  for convenience. In doing this, the potential  $V_{LR}$  was defined (see caption of Figure 1).

The wave packet is obtained, for different values of coordinate  $z$  by forming the expression:

$$\Psi(z, t) = \int_{-\infty}^{\infty} dp_R f(p_R - p_{Ro}) \psi_o(z, p_R, t), \quad (3)$$

where function  $f(p_R - p_{Ro})$  is a shape function which peaks at the value  $p_{Ro}$  and rapidly goes to zero for large values of the difference  $p_R - p_{Ro}$ , then the integral limits can be extended to  $\pm\infty$ .

In the case of the transmitted wave, taking  $D(p_R) \equiv 1$  as a condition of normalization of the wavefunction used to form the wave packet, one obtains for  $\Psi_R(z, t)$  for  $z$  in region  $R$ :

$$\Psi_R(z, t) = \int_{-\infty}^{\infty} dp_R f(p_R - p_{Ro}) B(p_R) \mathbf{e}^{\{i(zp_R/\hbar) + i\phi_t(p_R) - i(E(p_R))t/\hbar\}}. \quad (4)$$

The normalization condition means that the incident wave to form the packet is normalized in the  $L$  region. Here it was written  $A(p_R) \equiv B(p_R) \mathbf{e}^{i\phi_t(p_R)}$  using  $\phi_t(p_R)$  as the phase of the transmitted wave amplitude. For the case  $N \geq 2$  (*i. e.* a physical system described by two or more coupled differential equations), the condition of normalization have to be released because it is necessary to write the spinor as a part of the wave function.[25] In parameter  $A(p_R)$  the matching of the different layers in the structure is included. For  $N \geq 2$  this parameter is a vector, then this matching process appears in the coefficient  $B(p_R)$  and in the phase  $\phi_t(p_R)$  which in the multiband case must be calculated by components and no matrix expression can be given.

Considering the SPM to perform the integral in the case  $N = 1$  one has to expand in Taylor's series the exponent in (4) (which we called  $\Theta_T(p_R)$ ) and taking the value of  $p_R$  which produces an extreme for the exponent ( $p_{Ro}$ ) as the approximation, one obtains:

$$\Theta_T(p_R) = i(zp_R/\hbar) + i\phi_t(p_R) - i(E(p_R))t/\hbar. \quad (5)$$

The definition of the exponent

$$\Theta_T(p_{Ro}) \approx i(zp_{Ro}/\hbar) - i(E(p_{Ro}))t/\hbar + i\phi_t(p_{Ro}) + O(p_{Ro}^2) + \dots \quad (6)$$

The Taylor series up to second order,

$$\Psi_R(z, t) = G(p_{Ro}) \mathbf{e}^{i[-(tE(p_{Ro})/\hbar)' + (zp_{Ro}/\hbar)]} \mathbf{e}^{i(\phi_t(p_{Ro}) + \pi/4)} \quad (7)$$

The leading term of the wave packet,

$$G(p_{Ro}) = \frac{\sqrt{2\pi}B(p_{Ro})}{\left[ (d^2\phi_t(p_R)/dp_R^2)_{p_{Ro}} - [1/(m^*v_{gR})] (d\phi_t(p_R)/dp_R)_{p_{Ro}} \right]} \quad (8)$$

The coefficient of the leading term of the wavepacket.

Here we have considered that  $f(p_{Ro} - p_{Ro}) = 1$  and we use  $v_{gR}$  as the group velocity of the packet in layer  $R$ . Expression (7) is the leading term of the transmitted wavefunction, obtained by making this approximation. The coefficient of this wavefunction is given by (8) written in terms of the phase delay of the transmitted wave.

The applicability of the SPM takes into account that it uses the Taylor expand of the exponent and neglects the terms from the second order. This leads to write:

$$\Theta_T(p_R) = \Theta_T(p_{Ro}) + \Theta'_T(p_{Ro})(p_R - p_{Ro}) + \frac{1}{2}\Theta''_T(p_{Ro})(p_R - p_{Ro})^2 + \dots \quad (9)$$

$$\Theta_T(p_R) = \Theta_T(p_{Ro}) + \frac{1}{2}\Theta''_T(p_{Ro})(p_R - p_{Ro})^2 + \dots; \quad \text{as is an extreme.} \quad (10)$$

$$\frac{\Theta'''_T(p_{Ro})(p_R - p_{Ro})^3}{\Theta''_T(p_{Ro})(p_R - p_{Ro})^2} = \frac{\Theta'''_T(p_{Ro})(p_R - p_{Ro})}{\Theta''_T(p_{Ro})} < \epsilon; \quad \text{with } \epsilon \rightarrow 0. \quad (11)$$

Evaluating the derivatives of the exponential phase (11) in terms of the derivatives of the phase of the transmitted wave one obtains as the condition for the applicability of the SPM the expression:

$$\Sigma(p_R) = \frac{\hat{\Omega}_n(p_R)}{\hat{\Omega}_d(p_R)} = \frac{\left| \left( \frac{d^3 \phi_t(p_R)}{dp_R^3} \right)_{p_R=p_{Ro}} \right|}{\left| -\frac{1}{p_{Ro}} \left( \frac{d\phi_t(p_R)}{dp_R} \right)_{p_R=p_{Ro}} + \left( \frac{d^2 \phi_t(p_R)}{dp_R^2} \right)_{p_R=p_{Ro}} \right|^{3/2}} \ll 1. \quad (12)$$

This is the main contribution of this paper. This condition evaluates the applicability of the SPM and points over the use of the phase delay time for every group of values of the parameters of the system.

Nevertheless, this expression (12) has the numerator and the denominator dimensional and the quotient non dimensional, then to properly compare these expressions it is better to multiply by  $p_{Ro}^3$  both, numerator and denominator. This lead us to:

$$\Sigma(p_R) = \frac{\hat{\Omega}_n(p_R) \cdot p_{Ro}^3}{\hat{\Omega}_d(p_R) \cdot p_{Ro}^3} = \frac{\Omega_N(p_R)}{\Omega_D(p_R)} \quad (13)$$

$$\Omega_N(p_{Ro}) = \left| p_{Ro}^3 \left( \frac{d^3 \phi_t(p_R)}{dp_R^3} \right)_{p_R=p_{Ro}} \right| \quad (14)$$

$$\Omega_D(p_{Ro}) = \left| -p_{Ro} \left( \frac{d\phi_t(p_R)}{dp_R} \right)_{p_R=p_{Ro}} + p_{Ro}^2 \left( \frac{d^2 \phi_t(p_R)}{dp_R^2} \right)_{p_R=p_{Ro}} \right|^{3/2} \quad (15)$$

The phase time for the transmitted wave is obtained from the condition of stationary phase of the exponential in the integral (4). After including the matching at layer boundaries, one has for the

phase of the exponential in (7) the expression:

$$\alpha_T(p_R, t) = \frac{zp_R}{\hbar} + \phi_t(p_R) - \frac{t}{\hbar}E(p_R), \quad (16)$$

$$\frac{d\alpha_T}{dp_R} = 0 \implies \tau_T = \frac{m^*\hbar}{p_{Ro}} \left( \frac{d\phi_t(p_R)}{dp_R} \right)_{p_R=p_{Ro}}; \quad (17)$$

which is the formula to evaluate the phase delay time of the transmitted wave.[3] In (16) was taken, as Bohm did in his book,  $z \equiv \Delta z = 0$  because it refers to the phase between group  $M$  of layers and layer  $R$ , *i. e.*, the wave packet reaches the same position, later than if there were no dispersion potential causing the wave to be reflected. In this sense, the phase of layer  $R$  differentiates, bearing a term that comprises wave packets evolution delay information. For the case of  $N \geq 2$  bands, the whole analysis cannot be generalized for the present scheme from the case  $N = 1$  because the step of converting a complex number from  $a + ib$  to  $\rho e^{i\phi}$  cannot be performed in matrix notation and one must pass to  $2N \times 2N$  components. Further investigation is required to write close expressions in this case. This is important because there are several problems described by the standard Sturm-Liouville  $N \times N$  differential equation system[23] of great practical interest. Models as that due to Bogoliubov for superconductor excitations description[26] could be treated as well.

A simple consideration of closeness between the phase-time model and the dwell time (within its phase-time probabilistic average formulation [27, 28]), dispose us to speculate that the requirement (12) should be readily suited to it, with minor changes. We are interested in comparing these two possible conditions to get light into the use of different times for tunnelling processes.

### III. RESULTS AND DISCUSSION

The application of this formal analysis to different physical systems allows one to determine whether the phase time can be applied to a given system and to obtain it from the wavefunction. As an illustration we applied this procedure to the case of a double barrier resonant structure device in *GaAs/AlGaAs* considering the parameters shown in Table I.

The potential of the system is depicted in Figure 2, where the extreme left and right layers were considered as metallized contacts, which are semiconductors (*GaAs*) with flat band and an electric field applied to the structure.

Using (17), after making the matching considering the differences of masses in each layer by using the TM algorithm,[23] the phase delay time has the behavior depicted in figure 3 as a function of

the energy of the incident wave.

Our results for the phase time depicted in Figure 3 are of the same order of magnitude of other calculations and the behavior of the phase time is as others achieved, as can be seen in table II for electrons and photons in similar system, reported elsewhere.[13, 29, 30, 31] Several methods were used by these authors, namely: lifetime,[29] dwell time,[29] Wentzel-Kramer- Brillouin (WKB) quasi-classical approximation[30] and phase time.[13] In the case of photons, the reported values correspond to  $1.5 \mu\text{m}$  optical pulse wavelength, propagating through double-barrier photonic band gap (FBG).[31] In this table are included some useful data as if there is applied electric field, if the results were achieved theoretical or experimentally and the model used to perform the calculation. The application of the SPM to this system is governed by expression (12) and in Figures 4 a, b, c, d and e are shown separately the numerator  $\Omega_N(p_R)/10^6$ , the denominator  $\Omega_D(p_R)/10^{14}$  and the quotient  $\Sigma(p_R)$  of the applicability condition (13) for different energy ranges. This is the main result of this paper, because the phase delay time approximation is already known, but (13) is not used to assure its application to different systems. It is easily seen that in all graphics  $\Omega_N$  is under  $\Omega_D$ , so the procedure and the phase delay time are valid for all the energy range of interest. Nevertheless, there is an isolated point, seen in figure 4e) that goes over unity, and makes the SPM and the phase delay time inapplicable.

This analysis allows to say that this definition of time is good enough for many useful analysis at all energy ranges.

As a conclusion we have calculated the phase delay time in a system of semiconductor layers, illustrating with the simple case of a DBRT system described by the Schrödinger equation with an electric field applied and some light about the applicability of this definition of time is given by considering the condition obtained for the use of the SPM in reaching the transmitted wave packet. It is clear that one has to apply the applicability condition in each case under study to assure that the phase delay time is good in the conditions of each concrete problem. It is also an interesting guess to extrapolate the applicability condition obtained (12) for the phase time, to the case of the dwell time in its probabilistic average formulation[27, 28] with minor changes.

Also in this paper some considerations were made to extend these formulae to the case of systems with  $N$  second order coupled differential equations in which some of the algebra must be done in matrix notation and other cannot. This application leads to individual results for each component separately and after that one can rebuild the matrices. Expression (12) is valid for each one of the components and must be obtained and evaluated individually. The application of these results to

the case of  $N$  second order differential equations is in progress.

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- [24] There are several definitions of TM. Normally we use three of them. One transferring the wavefunction and the derivative in a domain; other transferring the wavefunction and the linear form which must be continuous at the interfaces and finally one transferring the coefficients of the wavefunction in the representation of propagating modes. (See 23). In the present paper we use the first TM mentioned.
- [25] This problem is not trivial. Usually the multiband cases are taken by considering all components but one zero, which is a particular case. Our analysis (see Ref.[15]) usually releases this consideration and all components are non zero. One must put the coefficient of the incident wave in layer  $L$  as normalized only. This means that our incident wave is a combination of all components.
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TABLE I: Parameters of the DBRT considered in the calculation sketched in Figure 2

No	Parameter	Value
1	Barrier Height ( $V_1$ )	250 meV
2	Difference between the band edges of sides $L$ and $R$ ( $V_o$ )	40 meV
3	Barrier width $b = z_1 - a_1$	40 Å
4	Well Width $d = z_2 - z_1$	100 Å
5	$m_1^*$ in units of $m_o$	0.066
6	$m_2^*$ in units of $m_o$	0.8

TABLE II: Time scale for tunneling

System	Potential	Structure	Data Source	Resonance [eV]	Bias [meV]	Time	Value of Time [ps]
electrons	DBRT	$\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$	Teo. Ref[29]	0.05	-	life	5.7
electrons	DBRT	$\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$	Teo. Ref[29]	0.18	-	life	2.9
electrons	DBRT	$\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$	Teo. Ref[29]	0.05	-	dwell	5.7
electrons	DBRT	$\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}/\text{As}$	Teo. Ref[29]	0.18	-	dwell	2.9
electrons	DBRT	$\text{Ga}_{0.47}\text{In}_{0.53}\text{As}/\text{Al}_{0.48}\text{In}_{0.52}\text{As}$	Teo. Ref[30]	-	40	WKB	0.5
electrons	DBRT	$\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$	Teo. Ref[13]	0.11	-	phase	0.02
electrons	DBRT	$\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$	Teo. Ref[13]	-	-	phase	$\approx 0.02$
photons	FBG	mono-mode optical fiber	Exp. Ref[31]	-	-	traversal	180
photons	FBG	mono-mode optical fiber	Teo. Ref[31]	-	-	phase	300

## Figure Captions

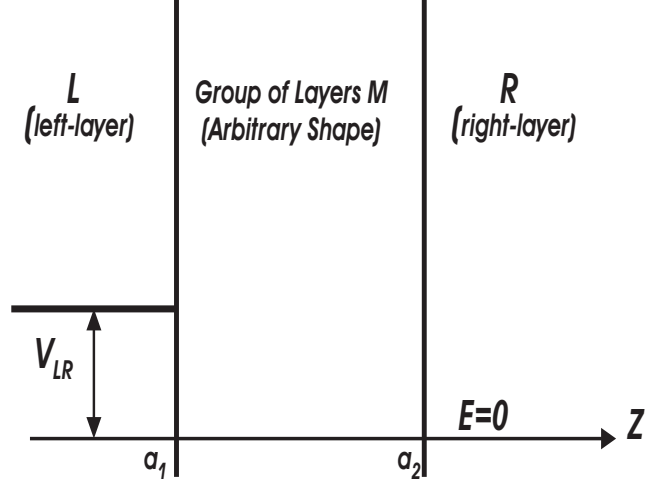


FIG. 1: General view of the Potential System under study. Layers  $L$  and  $R$  must not be equal necessarily.  $V_{LR}$  is the potential difference between the  $L$  band edge and the  $R$  band edge taken as energy reference level. In  $z$ -axis the interfaces are named as  $a_1$  and  $a_2$ .

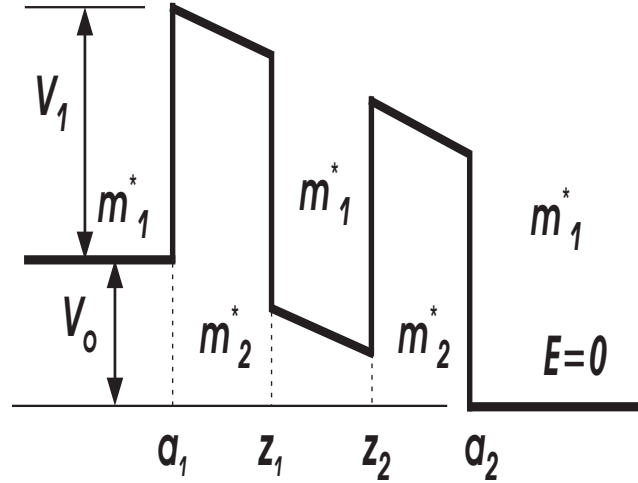


FIG. 2: General view of the DBRT system under study. Here  $V_o$  is called the  $V_{LR}$  of Figure 1. Points  $a_1$  and  $a_2$  are here the same as in Figure 1, then points  $z_1$  and  $z_2$  and potential  $V_1$  belong to layer  $M$  of Figure 1.

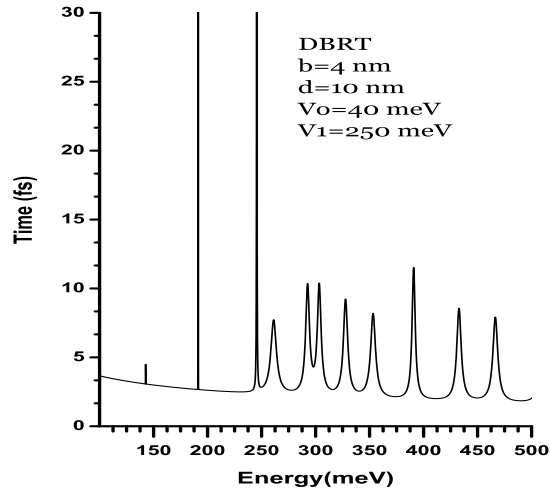
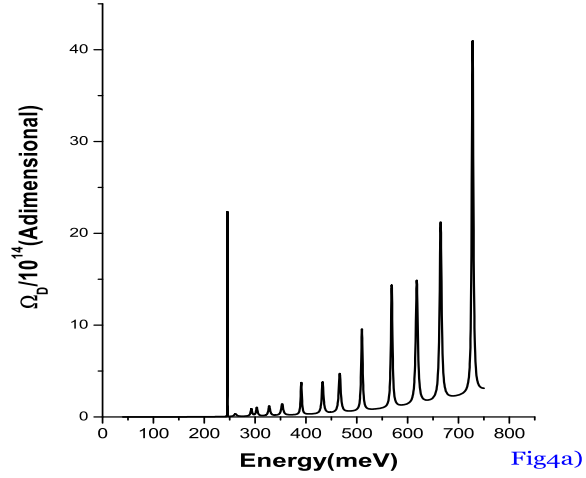
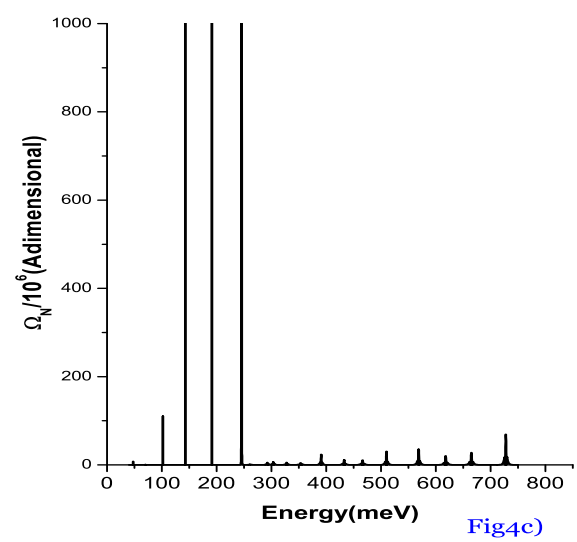
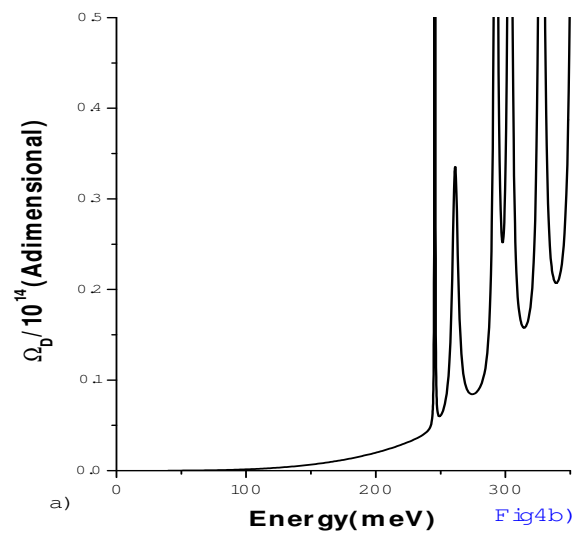


FIG. 3: Phase delay time calculated by (17) for the DBRT with the parameters given in Table I. For  $E < V_0$  the picks correspond to energies of the inner well.





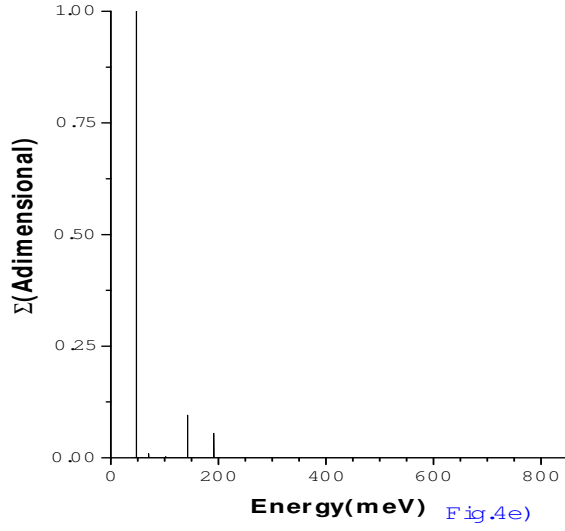
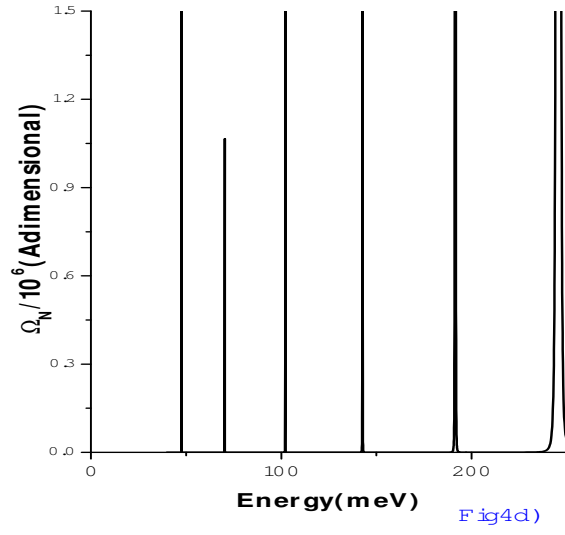


FIG. 4: Evaluation of the condition of applicability of the SPM (12) in the energy range. The shown graphs are: a) Denominator ( $\Omega_D(p_R)/10^{14}$ ) versus energy, b) The same as a) but in a particular energy range. c) Numerator ( $\Omega_N(p_R)/10^6$ ) vs energy, d) The same as c) but in a smaller energy range. and e) Quotient ( $\Sigma(p_R)$ ) versus energy in the whole energy range.